

## **Welcome to:**

# **The Agricultural and Food Chemistry NMR & NIR Micro-Spectroscopy Facility at the University of Illinois at Urbana-Champaign !**

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**Facility Coordinator: [Professor I.C. Baianu](#)**

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## **RELEVANT PUBLICATIONS:**

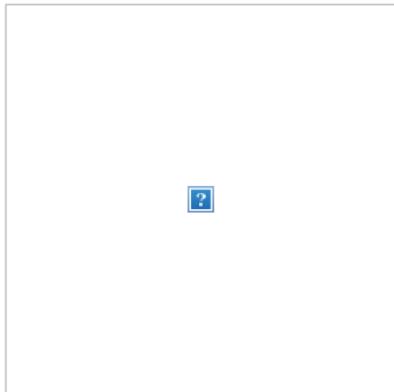
 [Chapter 5 "Spectroscopic Techniques for Studies of Food Systems with emphasis on Proteins.", I.C. Baianu and T.F. Kumosinski](#)

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 [Chapter 11: "Magnetic Resonance Studies of Pectin Polysaccharides in Apples: Hydration and Calcium-2+ Binding.", P. Irwin et al.](#)

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[Click on Image to see it Enlarged.](#)

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[3D Structure Determination by 2D-NMR: Image created in the group of Dr. Walter Chazin.](#)

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[View Large Image](#)



[View also the Large Image](#)

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"10 Minute Guide to HTML" by Tim Evans, Indiana: QUE publs., 1995.

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COMPUTER, Web-TERMS:  
("Hypertext Markup Language"=HTML= Web Language),

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URL address= "Uniform Resource Locator", or simply: -- an address on the Web--

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## News Release:

[NEW Link to the BioMagnetic Resonance Data Bank\('BioMagResBank'\), a valuable resource to the Magnetic Resonance researchers](#)

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[Important Global Forum and CONFERENCE on Soybeans: Contributed papers by February 4, 1999 \(see following two examples of spectroscopic applications to soybean analysis\)](#)

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HIGH-FIELD NMR AND NIR DETERMINATION OF OIL IN SOYBEANEMBRYOGENIC CELLS IN CULTURE

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NEAR INFRARED AND NUCLEAR MAGNETIC RESONANCE SPECTROSCOPYDETERMINATION OF PROTEIN, OIL, MOISTURE AND SUGAR CONTENTSIN SOYBEAN CULTIVARS

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ABSTRACT SUBMISSION PAGE

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# **The Fine Particle Society Symposium on NMR Applications in Food Science and Technology: March 31,1998 to April 3rd 1998, Dallas, The 'Monte Carlo' Hotel**

**FINAL PROGRAM:**

Symposium Chairman, Prof. I.C. Baianu, UIUC

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**SESSIONS: I. FINE**

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**PARTICLES IN FOOD PROCESSING:** Chair, Dr. I.C. Baianu, (UIUC)

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**PARTICIPANTS:** Dr. H.

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Cheng ( Hercules Inc.), T. Yates( The Dallas Group of America, Jeffersonville), Prof. E.G. Perkins (UIUC), Dr. P. I. Yakubu, PTI, St. Louis, MO, D. Costescu, UIUC, Dr. E. Ozu,(UIUC )

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- 1. H.N. Cheng, P. J. Cowan, L. J. Kasehagen (Hercules), "Modelling and Monte Carlo Simulation of Silicone-Carbon Resins"
- 2. D. Costescu, T. Yates, J.D. Caldwell, and I.C. Baianu. "Electron Microscopy and Monte Carlo Studies of Silica Gel Surface Structure."
- 4. Dr. P.I. Yakubu, PTI, ST. Louis, MO,(in collab. with Dr. E. Ozu): "NMR Studies of Potato Starch Hydration and Heat Processing of Potatoes from Selected Cultivars"

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**--- II. SOLID-STATE NMR TECHNIQUES/APPLICATIONS TO FOODS & PROCESSING & FINE PARTICLES:**  
Chair: Dr. Gary Turner, Director, Spectral Data Services. Inc., Urbana, Illinois;

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**----- PARTICIPANTS:**

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Dr. I.C. Baianu, UIUC; Dr. Jonathan Bass, PQ Corp., T. Yates, The Dallas Group of America

1. Ting Tao, Herman Lock and Gary E. Maciel." Some Recent Studies of the Silica Surface"  
 2. E.G. Perkins, T. Yates, and I.C. Baianu." CP-MAS and FT-IR Studies of Fatty Acid Adsorption on Magnesium Silicate Particles."

----- 3. Dr. G. Turner( Spectral Data Services): "High-resolution, Solid-State NMR of Silicates and Zeolites"  
 ----- 4. Dr. J. Shore (S. Dakota Univ.): 'Two-Dimensional and Double-Resonance Silicon-29 NMR Spectroscopy of Minerals'. 5. Dr. J. Bass (PQ), FTIR, Raman and Si-29 NMR Spectroscopy of Silicate Solutions

III. NMR OF SILICON POLYMERS. CHAIR: Dr. H.N. Cheng. (Hercules, Inc, USA.)

PARTICIPANTS: D. Costescu,C. Costescu (UIUC), Dr. Garry Turner, Dr. H.N. Cheng, Dr. J. Bass, Dr. M.J. Sullivan 1.Dr. M. J. Sullivan (Hercules Inc.) "Solution and Solid State NMR Characterization of Silicone-Carbon Resins."

----- 2.D. Costescu, C. Costescu,( in collab with T. Yates & J. D. Caldwell, The Dallas Group of America , and Prof. I.C. Baianu, UIUC): "Si-29 MASS, NMR- and Temperature Programmed Desorption Studies of Silicagels."

3. Dr. Garry Turner (Spectral Data Services, Inc.,and Dr. J. Bass, The PQ Corp.: "High-resolution NMR and FT-IR of Silicon Polymers in Solution."

4.Dr. Y. Kawakami (Japan Adv. Inst. of Sci.& Technol.) "Synthesis and Characterization of Optically Active Silicon-Containing Polymers".

IV. APPLICATIONS OF MAGNETIC RELAXATION TECHNIQUES IN FOODS and BIOMEDICAL SYSTEMS.

Chair: Dr. Robert Clarkson, UIUC, Vet. Biosciences & Illinois EPR Facility: email address: [clarkson@uiuc.edu](mailto:clarkson@uiuc.edu)

PARTICIPANTS:

----- Dr. Paul Cornillon, Purdue Univ., Dr.I.C. Baianu, UIUC,

1. Dr. R. Clarkson et al.: "Recent Advances in Spin Relaxation Studies of Biopolymers. ", (to be confirmed)

2. A. Mora-Gutierrez and I.C. Baianu (UIUC): "NMR relaxation studies of Myosin Activity in Concentrated Electrolyte Solutions."

3. Dr. Paul Cornillon (Purdue Univ.): 'NMR Relaxation Studies of Selected Food Systems."( to be confirmed)

V. NMR Applications in Foods and Q.C., CHAIR: Dr.I.C. Baianu, UIUC, FSHN (ACES Coll.) & Nuclear Engineering Depts.

----- Participants:

----- Dr. P.I. Yakubu, Protein Technology, Inc, St. Louis; Dr. E. Ozu, Osaka, JAPAN,

1.Dr. A. Mora-Gutierrez,( Prairie-View, University of Texas, Dallas): "NMR of Casein Hydration and Activity in Solutions with Ions."

2. Dr. T.F. Kumasinski( USDA, Eastern Regional REs. CENTER, Philadelphia, PA) , title to be announced 3. Dr. T.C. Wei ,( Natl. Food Res. Institute, Taiwan): NMR and Rheological Studies of Soy Protein Interactions with Water and Electrolytes in Relation to Food Processing."

4.Dr. J.R. Lee, (Natl. Res. Inst., Seoul, KOREA); "NMR Studies of Myofibrillar Proteins in Relation to Surimi Food Analogues".

----- VI. NMR OF FOOD BIOPOLYMERS AND GLASS TRANSITION:

Chair: Dr. Pavinee Chinachoti, University of Massachusetts at Amherst, Dept. of Food Science & Technology

Participants:

Dr. H.N. Cheng, Dr. I.C. Baianu, UIUC

1. Dr. P. Chinachoti:" NMR and DSC of Glass Transition in Hydrated Starch Systems and Doughs."

2. Dr. P.I. Yakubu, PTI, (in collab. with Dr. I.C. Baianu)."Deuterium and Carbon-13 CP-MASS NMR of Hydrated Potato Starch."

**VII. MRI of Food Systems.****CHAIR:**

1.Dr. Paul Cornillon, Purdue Univ.: "MRI of Food Doughs during Processing"  
3. Dr.E. Ozu, in collab. with Prof. I.C. Baianu): "NMR Studies of Water Distribution and Solid Matrix Changes in Selected Cultivars of Pumpkin during their Development."

----- SYMPOSIUM Chairman: Professor I.C. Baianu, UIUC

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**OLD ANNOUNCEMENTS:**

----- **The Fine  
Particle Society Symposium on NMR Applications in  
Food Science and Technology: August 7 and 8, 1996,  
Chicago, Hyatt Regency O'Hare Hotel , beginning 8:00  
AM, two sessions each day**

**NMR Applications to Food Biopolymers****FINAL PROGRAM:**

A SYMPOSIUM ON NMR APPLICATIONS IN FOOD SCIENCE AND TECHNOLOGY Thursday , August 8, 1996, Sessions I and II

Organizer and Chairman : I.C. Baianu , University of Illinois at Urbana-Champaign, Illinois

Co-Chairman: STATE-OF-THE-ART TECHNIQUES: R. Clarkson, Veterinary Medicine Dept. and the Illinois EPR Research Center, UIUC, Illinois

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**NMR APPLICATIONS TO FOOD BIOPOLYMERS AND OTHER SYSTEMS: Thursday: 8:00 AM - 11:00 AM**

1.Overview of NMR Applications to Food Biopolymers,

I.C. Baianu, University of Illinois at Urbana, IL

2. NMR Relaxation studies of surimi analogs: Starch and Muscle

Protein Hydration Determination,

P. Bechtel, Colorado State University, FSHN Dept, Fort Collins, CO, and P.H. Yakubu, University of Illinois at Urbana, AFC-NMR Facility, ACES College, Urbana, IL

3. Multi-Frequency EMR and NMR Studies of Lipid-Water Environments

R. B. Clarkson, A. Smirnov, T. Smirnova, Y. Chang, and

R.L. Belford, Depts. of Chemistry, Medicine, Veterinary Medicine,  
and the Illinois EPR Research Center, Urbana, IL 61801.

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**4. ROUND TABLE DISCUSSION:**

NMR Analysis of Foods and Related Model Systems

----- All interested FPS members are invited to participate in the informal, open discussions

STATE-OF-THE-ART TECHNIQUES AND MAGNETIC RESONANCE IMAGING  
DEVELOPMENTS with a View to Future Applications to Foods

Thursday , August 8, 1996, 1:30 PM to 3:30 PM

1. Magnetic Resonance Microscopy:Basic Principles and Applications

Doug Morris, University of Illinois at Urbana, Biomedical Magnetic Resonance Lab., 1307 W. Park St., Urbana, IL 61801.

2. Super-Resolution Image Reconstruction Dynamic MR Imaging,

Z.-P. Liang, University of Illinois at Urbana, IL.

3. Recent Developments and Applications of NMR Micro-coils,

J.Stocker and R. Magin, Beckman Research Institute for Advanced Studies, University of Illinois at Urbana.

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I.C. Baianu, Chair

## **Thursday Sessions: ABSTRACTS:**

### **Morning Session:**

#### **\*\*\*\*\* A SYMPOSIUM ON NMR APPLICATIONS IN FOOD SCIENCE AND TECHNOLOGY**

**Thursday , August 8, 1996, Sessions I and II**

**Organizer and Chairman : I.C. Baianu , University of Illinois at Urbana-Champaign, Illinois**

**NMR APPLICATIONS TO FOOD BIOPOLYMERS AND OTHER SYSTEMS:**

**Thursday: 8:00 AM - 11:00 AM**

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#### **Overview of NMR**

#### **Applications to Food Biopolymers.**

**I.C. Baianu, University of Illinois at Urbana, Illinois 61801**

**A comprehensive survey of NMR techniques and their selective applications for the characterization of food biopolymers and related model systems will be presented. Both high-resolution and relaxation aspects of NMR applications to foods will be discussed, emphasizing the practical and potential uses of NMR in the food industry. Specific applications for a variety of foods and model systems will be illustrated at an intuitive and accessible level to the food processing engineer and R&D specialists. Other results recently obtained at the Agricultural & Food Chemistry NMR Facility in the ACES College at UIUC can be previewed on the Internet at the following URL addresses:**

**<http://www.ag.uiuc.edu/~fs401/AFC-NMR-FACILITY.html>**

**, <http://www.ag.uiuc.edu/~fs401/FS-401-96-UPDATE.html> ,**

**and <http://www.ag.uiuc.edu/~fs401/Adv-antiox.html>**

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#### **NMR Relaxation studies of Surimi Analogs: Starch and Muscle Protein**

**Hydration Determination.**

**P. Bechtel, Colorado State University, FSHN Dept, Fort Collins, CO, and P.H. Yakubu, University of Illinois at Urbana, AFC-NMR Facility, ACES College, Urbana, IL** Recent NMR relaxation results for surimi analogs made of heart or gizzard muscle proteins with potato starches from selected cultivars will be presented and discussed in relation to developing novel food formulations. Determination of both hydration and structural changes in these food systems as a result of various thermal processing methods will be presented, and shown to be relevant to quality control and functionality in foods. -----

**Multi-Frequency EMR and NMR Studies of Lipid-Water Environments.**

**R. B. Clarkson, A. Smirnov, T. Smirnova, Y. Chang, and R.L. Belford, Depts. of Chemistry, Medicine, Veterinary Medicine, and the Illinois EPR Research Center, Urbana, IL 61801.**

Organic chelates of paramagnetic metal ions can be designed to exhibit various degrees of lipophilicity. The chemistry of these materials is of special interest to researchers who are designing paramagnetic MRI contrast agents with tissue-specific properties that can be exploited in both nutritional and medical diagnostic investigations. We are reporting the use of field-cycling NMR relaxometry, as well as multi-frequency EMR techniques to characterize the environment, dynamics, and water interactions of the chelates. In this paper, we will present results from novel 2-dimensional NMRD studies of Gd(III) chelates interacting with albumins and primary rat hepatocytes, as well as complementary EMR studies at frequencies from 1 to 250 GHz that relate to the presence of unpaired electrons in these systems. Changes in the rotational motion of the complexes, as well as in their effective "g-values" occur when such molecules interact with lipids. Partitioning effects are sometimes observable in the 2-dimensional NMRD profiles when water and paramagnetic chelate exchange rates are favorable. The new frequencies available for EMR studies have many potential applications in the characterization of membrane properties utilizing paramagnetic spin probes. Our novel methodology could therefore be applied, for example, to determine both eukariotic and prokariotic cell membrane fluidity. This work was supported in part by grants from the NIH (GM42208,

**GM51630, to RBC; RR01811 to RLB), and by Schering AG , and Nycomed AB. Use of the facilities of the Illinois EPR Research Center, an NIH-supported national research resource center, is gratefully acknowledged.** -----

**ROUND TABLE DISCUSSION: NMR Analysis of Foods and Related Model Systems (All symposium participants) An informal discussion of the latest developments of both applications and methodology for Food Analysis, with emphasis on Food Chemistry, Engineering and Nutrition areas.**

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**Afternoon Session: STATE-OF-THE-ART TECHNIQUES: Chair: I.C. Baianu, AFC-NMR Facility, UIUC, Illinois Session Co-Chairman R. Clarkson, Veterinary Medicine Dept. and the Illinois EPR Research Center, UIUC, Illinois STATE-OF-THE-ART TECHNIQUES AND MAGNETIC RESONANCE IMAGING DEVELOPMENTS with a View to Future Applications to Foods. Thursday , August 8, 1996, 1:30 PM to 3:30 PM ----- Magnetic**

**Resonance Microscopy: Basic Principles and Applications D. Morris, Biomedical Magnetic Resonance Laboratory, University of Illinois at Urbana, 1307 W. Park. St., Urbana, IL. 61801 An overview of recent advances in Magnetic Resonance Microscopy will be presented with special emphasis of potential applications of these novel techniques to the characterization of foods and biological systems, in general. Specific illustrations will be shown to bring several important applications into focus.** ----- Super-

**resolution, MR Imaging with A Priori Constraints Z.-P. Liang, Department of Electrical and Computer Engineering and Beckman Institute for Advanced Science and Technology, Urbana, IL. 61801 A classical problem with tomographic imaging is the so-called limited data reconstruction problem which occurs when physical and temporal constraints prevent sufficient coverage of the data space. Traditionally, image reconstruction is performed using the Fourier series model, which often results in spurious ringing, loss of spatial resolution, and motion artifacts. To overcome these problems, numerous methods have emerged in the past decade to incorporate a priori information into the imaging process. This paper is devoted to a discussion of the constrained imaging**

**concept. Specifically, three model-based imaging methods will be discussed to illustrate how a priori constraints can be used to achieve super-resolution image reconstruction, to improve imaging efficiency with time-sequential imaging, and to suppress motion artifacts and improve temporal resolution with dynamic imaging.** -----

----- **Recent Developments and Applications of NMR Micro-coils. J.Stocker and R. Magin, Beckman Research Institute for Advanced Studies, University of Illinois at Urbana, Illinois** A fundamental limitation in NMR micro-spectroscopy is the low signal-to-noise ratio (SNR). Microcoils, with diameters on the order of 500 micrometers or less, have been shown to provide enhanced sensitivity for RF detection from mass-limited and volume-limited samples. With solenoid microcoils, a SNR (per acquisition) higher than 100:1, and linewidths less than 1 Hz have been obtained. Such microcoils are employed for capillary electrophoresis --NMR, and liquid chromatography-- NMR. At dimensions of less than 100 micrometers, microlithographic fabrication techniques are now being employed to make planar microcoils (spiral inductors). With such planar microcoils, experimental results were obtained with SNR values of 25:1, and linewidths less than 2 Hz. These results demonstrate the application of these microcoils to high resolution microspectroscopy, and represent a critical component in the development of microcoil arrays, integrated pre-amplifiers, and eventually integrated NMR detectors.